THE GEOMETRY OF POINT PARTICLES

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Abstract

There is a very natural map from the configuration space of n distinct points in Euclidean 3-space into the flag manifold $U(n)/U(1)^n$, which is compatible with the action of the symmetric group. The map is well-defined for all configurations of points provided a certain conjecture holds, for which we provide numerical evidence. We propose some additional conjectures, which imply the first, and test these numerically. Motivated by the above map, we define a geometrical multi-particle energy function and compute the energy minimizing configurations for up to 32 particles. These configurations comprise the vertices of polyhedral structures which are dual to those found in a number of complicated physical theories, such as Skyrmions and fullerenes. Comparisons with 2-particle and 3-particle energy functions are made. The planar restriction and the generalization to hyperbolic 3-space are also investigated.

1 Introduction

In their study of the spin-statistics theorem, Berry and Robbins [5] posed a very natural question in classical geometry concerning the existence of a symmetric map between two well-known spaces. The first space, denoted by $\mathcal{C}_n(\mathbb{R}^3)$, is the configuration space of n distinct ordered points in $\mathbb{R}^3$, and the second space is the flag manifold $U(n)/U(1)^n$, an element of which represents n orthonormal vectors in $\mathbb{C}^n$, each defined up to a phase. The Berry-Robbins problem is to construct, for each n, a continuous map

$$f_n : \mathcal{C}_n(\mathbb{R}^3) \mapsto U(n)/U(1)^n \tag{1.1}$$

compatible with the action of the symmetric group Σ_n, where this acts freely by permuting the points and the vectors respectively.

In the application of Berry and Robbins an element of $\mathcal{C}_n(\mathbb{R}^3)$ represents the positions of n point particles and the matrix $U(n)$ describes how a spin basis varies as the points move in space. In this approach to the spin-statistics theorem the Pauli sign associated with the exchange of particles arises as a geometric phase.

For the simplest case, $n = 2$, there is an obvious explicit map as noted by Berry and Robbins [5] but this construction is difficult to generalize to $n > 2$. A candidate solution for all n was first presented in [1], and is reviewed in Section 2. The map is only a candidate solution because it relies upon a certain non-degeneracy conjecture being true. Section 3 introduces an appropriate determinant function (whose non-vanishing describes the non-degeneracy) which can be used in subsequent quantitative investigations. In Section 4 we provide numerical evidence for the validity of this conjecture and propose and test numerically some additional conjectures, which imply the first.

Motivated by the construction of the above map, we define, in Section 5, a geometrical multi-particle energy function and compute the energy minimizing configurations for up to 32 particles. Remarkably, the resulting configurations of points comprise the vertices of polyhedral structures which are dual to those found in a number of complicated physical theories, including Skyrmions in nuclear physics and fullerenes in carbon chemistry. These results suggest a comparison, made in Section 6, with the historic problem concerning the minimal energy distribution of n point charges on the surface of a sphere, interacting via a 2-particle Coulomb force. In Section 7 we propose an approximation to our multi-particle energy function in terms of a 3-particle interaction, and find essentially the same minimal energy configurations.

The remaining sections concern minimal energy configurations in various modifications of the above picture. In Section 8 we enlarge the configuration space to consider unconstrained points in a product of spheres and show that the minimal energy configurations remain unchanged. In Section 9 we consider the restriction to points in the plane and repeat our earlier comparisons. Finally, in Section 10, we generalize the whole situation to hyperbolic 3-space.

2 The map

A candidate map for f_n in (1.1) was first presented in [1], to which we refer the reader for further details. Below we summarize the main ingredients.

First of all, any set of n linearly independent vectors in $\mathbb{C}^n$ can be orthogonalized, in a way compatible with Σ_n, so the unitarity condition in (1.1) can be relaxed to require a map

$$F_n : \mathcal{C}_n(\mathbb{R}^3) \mapsto GL(n,\mathbb{C})/(\mathbb{C}^*)^n \,. \tag{2.1}$$

Given $(\mathbf{x}_1,\ldots,\mathbf{x}_n) \in \mathcal{C}_n(\mathbb{R}^3)$ then (2.1) is equivalent to defining n points $p_i(\mathbf{x}_1,\ldots,\mathbf{x}_n) \in \mathbb{CP}^{n-1}$, for $i = 1,\ldots,n$, which are linearly independent. We shall represent $\mathbb{CP}^{n-1}$ via the space of polynomials of degree at most $n-1$ in a Riemann sphere variable $t \in \mathbb{CP}^1$.

The explicit map is constructed as follows. For each pair $i \neq j$ define the unit vector

$$\mathbf{v}_{ij} = \frac{\mathbf{x}_j - \mathbf{x}_i}{|\mathbf{x}_j - \mathbf{x}_i|} \tag{2.2}$$

giving the direction of the line joining $\mathbf{x}_i$ to $\mathbf{x}_j$. Now let $t_{ij} \in \mathbb{CP}^1$ be the point on the Riemann sphere associated with the unit vector $\mathbf{v}_{ij}$, via the identification $\mathbb{CP}^1 \cong S^2$, realized as stereographic projection. Finally, set p_i to be the polynomial in t with roots t_{ij} $(j \neq i)$, that is

$$p_i = \prod_{j\neq i}(t - t_{ij}) \,. \tag{2.3}$$

The geometrical character of this construction means that, in addition to the required compatibility with Σ_n, the map is also compatible with rotations in $\mathbb{R}^3$, where $SO(3)$ acts as the irreducible n-dimensional representation on the target space. Furthermore, the map is also translation and scale invariant; this follows trivially from (2.2).

The reason that this map is only a candidate solution is that the following conjecture must hold.

Conjecture 1
For all $(\mathbf{x}_1,\ldots,\mathbf{x}_n) \in \mathcal{C}_n(\mathbb{R}^3)$ the polynomials $p_1,\ldots,p_n$ are linearly independent.

For $n = 2$ this conjecture is trivially true and for $n = 3$ it can be proved using simple geometry [1] or a direct algebraic computation [2], which we mention in the following section.

Note that an obvious case to check is that of n collinear points. Taking the line of collinear points to be in the direction given by $t = \infty$ and ordering the $\mathbf{x}_i$ in increasing distance along the line yields $p_i = t^{i-1}$, which are clearly independent.

For $n > 3$ the conjecture remains open. In Section 4 we provide numerical evidence for this conjecture, and for some related conjectures which imply this one. Before this, we discuss a determinant function which will prove useful in making quantitative investigations, and which turns out to have independent interest, as we shall show. Because of this we shall treat it in greater generality than is needed for our immediate purposes. Readers interested in the main results of our numerical calculations can skip the details of the next section.

3 Determinant functions

Linear independence can be characterized by the non-vanishing of the appropriate determinant. Because the polynomials $p_1,\ldots,p_n$ in conjecture 1 are only defined up to scalar factors we have to introduce an appropriate normalization if we want a definite determinant. There are several ways in which this can be done. One way is described in detail in [2]: for the absolute value of the determinant one just takes each p_i to have norm 1 and then takes the volume in $\mathbb{C}^n$ given by the essentially unique $SU(2)$-invariant inner product. The phase requires more careful treatment as explained in [2]. There is however an alternative approach, which we shall adopt here, that has a number of advantages. On the one hand, as already exhibited in [2] this new definition has much better quantitative behaviour, and this we shall be exploiting in our numerical calculations. Another and apparently quite different advantage lies in the fact that this new definition extends naturally to hyperbolic 3-space and hence, on lines forecast in [2], to Minkowski space.

We start as follows. Consider $n(n-1)$ variables $u_{ij} \in \mathbb{C}^2$ $(i \neq j)$ $i, j = 1, 2, \ldots, n$, and form the n 'polynomials' $p_1, \ldots, p_n$ given by

$$p_i = \prod_{j \neq i} u_{ij}. \tag{3.1}$$

This is a more abstract version of (2.3), where u_{ij} is regarded as a linear form

$$u_{ij} = a_{ij} t_0 + b_{ij} t_1 \tag{3.2}$$

in two homogeneous coordinates (t_0, t_1) related to the inhomogeneous coordinate t of (2.3) by $t = t_0/t_1$.

If we want to avoid using coordinates, and hence emphasize the invariance, we consider $\mathbb{C}^2$ as a vector space with a skew non-degenerate form (u, v). In particular this identifies $\mathbb{C}^2$ with its dual, the space of linear forms. Note that $\mathbb{C}^2$ is the space of *spinors*.

In (3.1) p_i is just given by the symmetrized tensor product of n copies of $\mathbb{C}^2$

$$S^n(\mathbb{C}^2) \cong \mathbb{C}^n. \tag{3.3}$$

Since $SL(2, \mathbb{C})$ acts on $\mathbb{C}^2$ preserving the skew-form it acts (irreducibly) on $\mathbb{C}^n$ via $SL(n, \mathbb{C})$.

Now take the n vectors $p_1, \ldots, p_n$ in $\mathbb{C}^n$ and form the exterior product

$$\omega = p_1 \wedge p_2 \wedge \ldots \wedge p_n \tag{3.4}$$

which is an element of the nth exterior power of $\mathbb{C}^n$. Since there is a canonical isomorphism

$$\Lambda^n(\mathbb{C}^n) \cong \mathbb{C} \tag{3.5}$$

ω is essentially a complex number. More precisely

$$\omega = \varphi \; e_1 \wedge e_2 \wedge \ldots \wedge e_n \tag{3.6}$$

where e_i is the monic polynomial t^{i-1}, or in other words φ *is the determinant of the matrix of coefficients of the polynomials* $p_1, \ldots, p_n$. Our parameter t is assumed here to come from an orthogonal, or at least symplectic basis (t_0, t_1) of $\mathbb{C}^2$ (see the later discussion of symplectic representatives).

We have therefore defined a *complex-valued function* $\varphi(u_{ij})$. It has the following properties

(1) φ is invariant under the action of $SL(2, \mathbb{C})$ on the u_{ij}.

(2) $\varphi(u^*_{ij}) = \overline{\varphi(u_{ij})}$, where $(a + bt)^* = (-\bar{b} + \bar{a}t)$.

(3) $\varphi(u_{\sigma(i)\sigma(j)}) = \operatorname{sign}(\sigma)\varphi(u_{ij})$, for any permutation σ of $(1, \ldots, n)$.

(4) φ is a multi-linear function of the u_{ij}.

(5) For $n = 2$, $\varphi = (u_{12}, u_{21})$.

Remark: The essential difference between this definition and the earlier one in [2] is that here we do not use any Hermitian metric on $\mathbb{C}^n$, only the volume form. That is why we have the larger symplectic group $SL(2, \mathbb{C})$ rather than just $SU(2)$.

In terms of φ we can proceed to define a sequence of related functions φ_k (for $2 \leq k < n$), using subsets I of $(1, \ldots, n)$ of length $|I| = k$. For each such I let φ_I be the function φ applied to the variables u_{ij} with $i, j \in I$, and then put

$$\varphi_k = \prod_I \varphi_I, \quad |I| = k. \tag{3.7}$$

Thus we have the sequence of functions

$$\varphi = \varphi_n, \varphi_{n-1}, \ldots, \varphi_2. \tag{3.8}$$

Clearly from property (4) of φ we deduce

(6) φ_k is homogeneous in each u_{ij} of degree $\binom{n-2}{k-2}$.

If we take a ratio of appropriate powers of the φ_k then we will get a rational function of homogeneity zero in the u_{ij}. This means that it is a rational function of the corresponding points $t_{ij} \in P_1(\mathbb{C})$. In particular we shall be interested in

$$D(t_{ij}) = \varphi_n(u_{ij})/\varphi_2(u_{ij}). \tag{3.9}$$

Note that this has poles only where $\varphi_2(u_{ij}) = 0$, ie. where u_{ij} and u_{ji} are proportional, or equivalently where $t_{ij} = t_{ji}$. From now on *we restrict ourselves to the subspace of the variables where, for all i, j, $t_{ij} \neq t_{ji}$.*

A convenient way to make the definition of D more explicit is to use *symplectic representatives* for the u_{ij}. By definition this means that we choose each pair u_{ij}, u_{ji} so that (for $i < j$)

$$(u_{ij}, u_{ji}) = 1. \tag{3.10}$$

This makes $\varphi_2 = 1$ and so $D = \varphi$ is just the determinant of the coefficients of the polynomials $p_1, \ldots, p_n$.

If we introduce a Hermitian metric on $\mathbb{C}^2$, with $SU(2)$ now being the symmetry group we can introduce the anti-podal map

$$t \mapsto t^* = -\bar{t}^{-1} \tag{3.11}$$

and we can lift this to an anti-linear map $u \mapsto u^*$ on $\mathbb{C}^2$. Explicitly, in terms of a standard basis, this is (as in (2) above) $(a, b) \mapsto (-\bar{b}, \bar{a})$. If we think of $\mathbb{C}^2$ as the quaternions then $u^* = uj$. Note that

$$(u, u^*) = |a|^2 + |b|^2 = |u|^2 \tag{3.12}$$

so that if $|u| = 1$, the pair u, u^* are a symplectic pair. Such a pair we shall briefly refer to as an orthogonal pair (since $|u| = |u^*| = 1, < u, u^* >= 0$).

We are now ready to return to our configurations of points $\mathbf{x}_1, \ldots, \mathbf{x}_n$ in $\mathbb{R}^3$ and the corresponding points t_{ij} (or $\mathbf{v}_{ij}$) given by (2.2), ie. by the directions of the vectors $\mathbf{x}_j - \mathbf{x}_i$. Our function $D(t_{ij})$ then gives rise to a function $D(\mathbf{x}_i)$ on $\mathcal{C}_n(\mathbb{R}^3)$. Since our t_{ij} now satisfy $t_{ij} = t_{ji}^*$ we can choose orthogonal representatives for the u_{ij} and so we get D as the determinant of the coefficients of the polynomials $p_1, \ldots, p_n$.

In [2] we defined D explicitly in this way, except that we multiplied it by a numerical coefficient $\mu(n)$. This arose from using the invariant inner product on $\mathbb{C}^n$, but is not natural from our present more invariant point of view. We have therefore dropped it. Note however that the geometrical considerations in [2] led to an upper bound for $|D|$, which now becomes

$$|D| \leq \mu(n)^{-1} = \{\prod_{s=0}^{n-1} \binom{n-1}{s}\}^{1/2} \tag{3.13}$$

where $\binom{n-1}{s}$ is the binomial coefficient.

The whole purpose of introducing our function D is of course that conjecture 1 is equivalent to

$$D(\mathbf{x}_1, \ldots, \mathbf{x}_n) \neq 0. \tag{3.14}$$

Properties (1) and (2) show that, as a function $\mathcal{C}_n(\mathbb{R}^3) \mapsto \mathbb{C}$ it is covariant with respect to the full Euclidean group of $\mathbb{R}^3$, with reflections acting as complex conjugation on $\mathbb{C}$. This implies in particular that D is *real* for any *planar* configuration, which is automatic for $n = 2$ ($D = 1$) and $n = 3$. In general, for $n \geq 4$, D is complex and we shall introduce its norm

$$V = |D| \tag{3.15}$$

as a real-valued function on $\mathcal{C}_n(\mathbb{R}^3)$ and refer to it briefly as the *volume*. For any collinear set we have already noted that, in a suitable orientation, we have $p_i = t^{i-1}$ and so $V = 1$.

For $n = 3$ the calculation of the volume yields a nice geometrical answer [2]. Let the triangle formed by the three points $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$ have angles $\theta_1, \theta_2, \theta_3$, then

$$V = \frac{1}{2}[\sin^2(\frac{\theta_1+\theta_2}{2}) + \sin^2(\frac{\theta_2+\theta_3}{2}) + \sin^2(\frac{\theta_3+\theta_1}{2})]\,. \tag{3.16}$$

This formula is obtained by explicitly computing the polynomials p_i and using some elementary geometry.

Using the fact that $\sum_{i=1}^{3} \theta_i = \pi$ the critical points of V are easily determined as the solutions of

$$\sin\theta_1 = \sin\theta_2 = \sin\theta_3\,. \tag{3.17}$$

There are two classes of solutions. The first is $\theta_1 = \theta_2 = 0$ and $\theta_3 = \pi$, in which the triangle degenerates to three collinear points with $V = 1$. This is the global minimum of the volume. The second is the global maximum, given by the equilateral triangle $\theta_1 = \theta_2 = \theta_3 = \pi/3$, for which $V = 9/8$. Thus, V is non-zero for all configurations of three points and conjecture 1 is proved in the case $n = 3$.

For $n > 3$ conjecture 1 has yet to be proved. In the following section we make use of the volume function V to provide numerical evidence for this conjecture, and for some related conjectures which imply this one.